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Internal and external factors influencing the Diels-Alder reaction

Kiselev V., Konovalov A.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

The internal and external key factors influencing the reaction rates were considered for the Diels-Alder reaction (DAR) with normal electron demand. A simple dependence lgk2= -28.81+316.3/(IPD=E A-69.9 R1-4/(IPD-EA)-0. 054ΔHr-n for the reaction rate as a function of the ionization potential of π-donor dienes, electron affinity of π-acceptor dienophiles, heat of reaction and diene structure (R1-4) was obtained. This relation allows one to explain the origin of the conventional and 'anomalous' relations between activity and selectivity, and the variety of relationships between the kinetic activity and thermodynamic stability. It helps one to choose the conditions for the directed synthesis of desired products, to explain the acceleration effects in the presence of Lewis acids and to predict the rates of the DAR between the different reagents with C=C bonds not explored earlier. Copyright © 2009 John Wiley & Sons, Ltd.

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Keywords

Catalysis, Diels-Alder reaction, Factors determining reactivity, High pressure effect, P, p- and n, v-molecular complexes